STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 126155

TO: Ben Sackey **Location: rem/5b31/5c18** **Art Unit: 1626** **Wednesday, July 14, 2004** **Case Serial Number: 10/656867**	**From: Noble Jarrell** **Location: Biotech-Chem Library** **Rem 1B71** **Phone: 272-2556** **Noble.jarrell@uspto.gov**

Search Notes

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=> d his

     (FILE 'HOME' ENTERED AT 07:46:39 ON 14 JUL 2004)

     FILE 'REGISTRY' ENTERED AT 07:50:47 ON 14 JUL 2004
                ACT SAC867S1/A
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L1               STR
L2            36 SEA FILE=REGISTRY SSS SAM L1
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                 ACT SAC867PRO/A
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L3               STR
L4   (   1079943)SEA FILE=REGISTRY ABB=ON  PLU=ON  16.136/RID
L5            50 SEA FILE=REGISTRY SUB=L4 SSS SAM L3

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L8               STR L6.
L9             0 L8
L10              STR L8
L11            0 L10
L12              STR L10
L13              STR L10
L14            0 L13
L15              STR L13
L16            0 L15
L17              STR L15
L18            0 L17
L19        48256 NITRILE/FG.RCT OR NITRILE/FG.RGT
L20            0 L13 SAM SUB=L19
L21              STR L13
L22            0 L21
L23            3 L13 FULL SUB=L19
                 E PAGENKOPF B/AU
L24           16 E4
                 E YU MING/AU
L25           14 E3-5
                 E YU M/AU
L26            1 E3
L27          290 (DEP? (1A) CHEM? (1A) BIOC? (1A) UNIV? (1A) (TX OR TEXAS) (1A)
L28            8 L21 FULL
L29            1 (L23 OR L28) AND L24-26
L30            1 (L23 OR L28) AND L27
L31            1 L29-30
L32            7 (L23 OR L28) NOT L31
L33            7 L32 AND (PY<=2003 OR AY<=2003 OR PRY<=2003 OR AD<20030905 OR PD

     FILE 'REGISTRY' ENTERED AT 09:50:11 ON 14 JUL 2004
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L50           33 E4
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L51          453 E3-52
L52            4 (DEPT (1A) CHEM (1A) BIOC? (1A) UNIV? (1A) (TX OR TEXAS) (1A) A
L53            2 (DEPARTMENT (1A) CHEM (1A) BIOC? (1A) UNIV? (1A) (TX OR TEXAS)
L54           70 L49 (L) RACT+NT/RL
L55         4334 L48 (L) PREP+NT/RL
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L59            1 L56 NOT L57
L60            1 L59 AND (PY<=2003 OR AY<=2003 OR PRY<=2003 OR AD<20030905 OR PD

=> b casreact
FILE 'CASREACT' ENTERED AT 10:41:51 ON 14 JUL 2004
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FILE CONTENT:1840 - 11 Jul 2004 VOL 141 ISS 2

************************************************************
*                                                          *
*     CASREACT now has more than  8 million reactions      *
*                                                          *
************************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=> d que stat l23
L13              STR
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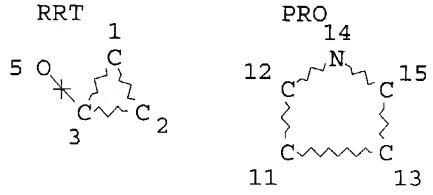


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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
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L23 3 SEA FILE=CASREACT SUB=L19 SSS FUL L13 (16 REACTIONS)

100.0% DONE 148217 VERIFIED 16 HIT RXNS 3 DOCS
SEARCH TIME: 00.00.06

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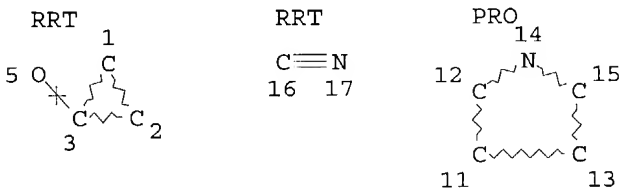
L21 STR



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NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE
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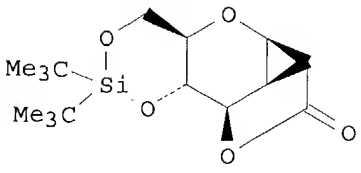
100.0% DONE 225002 VERIFIED 39 HIT RXNS 8 DOCS
SEARCH TIME: 00.00.11

=> d bib abs rx l31 tot

L31 ANSWER 1 OF 1 CASREACT COPYRIGHT 2004 ACS on STN
AN 139:164719 CASREACT
TI Formal [3 + 2] Cycloadditions of Donor-Acceptor Cyclopropanes and Nitriles
AU **Yu, Ming; Pagenkopf, Brian L.**
CS **Department** of **Chemistry** and **Biochemistry**,
University of **Texas**, **Austin**, TX, 78712, USA
SO Journal of the American Chemical Society (2003), 125(27), 8122-8123
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
GI



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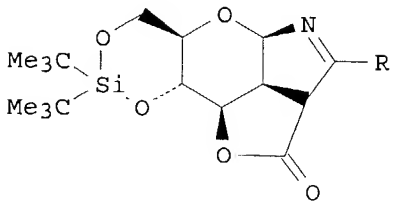
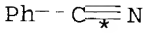


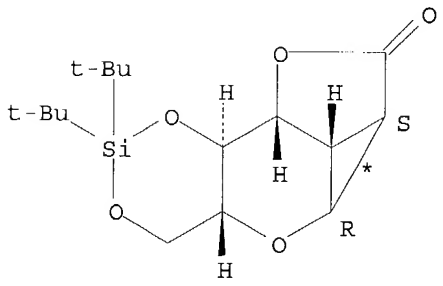
II

AB Upon activation with trimethylsilyl triflate, donor-acceptor cyclopropanes, e.g. I, cleave to give reactive intermediates that can be efficiently intercepted by nitriles RCN [R = Me, Ph, Me3C, PhCH:CH, MeOCH:CH, Cl(CH2)3, etc.] in a formal [3 + 2] dipolar cycloaddn. reaction to afford synthetically useful 2H-3,4-dihydropyrrole cycloaddn. products, e.g. II, in high yields.

RX(1) OF 13 **A** + **B** ===> **C**



A



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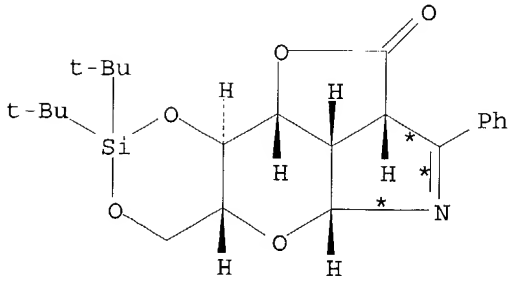


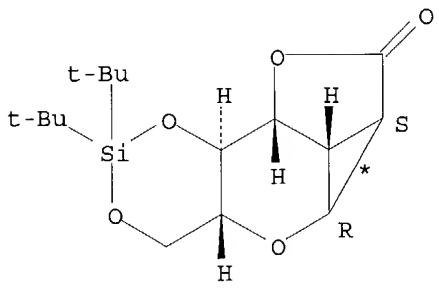
C
YIELD 81%

RX(1) RCT A **100-47-0**, B **361456-14-6**

RGT D 27607-77-8 Me3SiSO3CF3
PRO C **575444-66-5**
SOL 75-09-2 CH2Cl2

RX(2) OF 13 **F** + **B** ===> **G**

F



B

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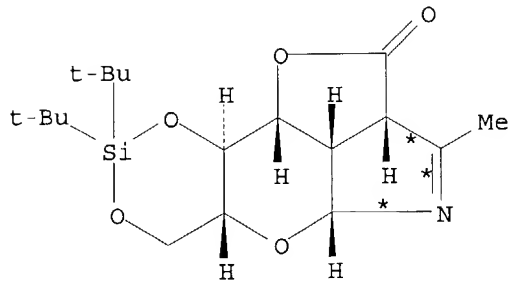
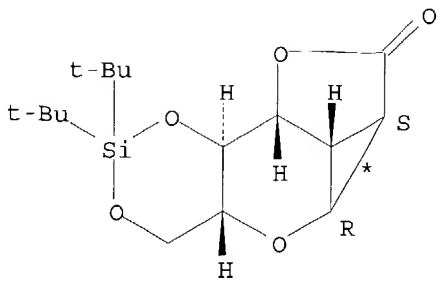


G
YIELD 96%

RX(2) RCT F **75-05-8**, B **361456-14-6**
RGT D 27607-77-8 Me3SiSO3CF3
PRO G **575444-67-6**
SOL 75-05-8 MeCN
NTE alternative prepn. shown

RX(3) OF 13 **B** + **H** ===> **I**



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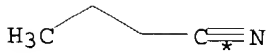

H

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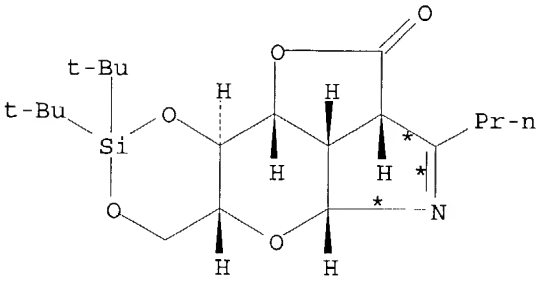
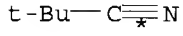


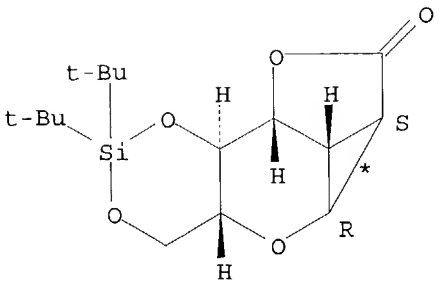
I
YIELD 95%

RX(3) RCT B **361456-14-6**, H **109-74-0**
RGT D 27607-77-8 Me3SiSO3CF3
PRO I **575444-68-7**
SOL 75-09-2 CH2Cl2

RX(4) OF 13 **J** + **B** ===> **K**



J



B

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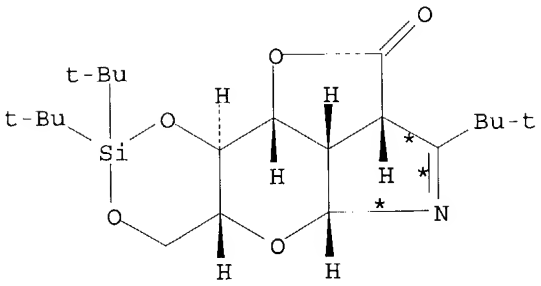
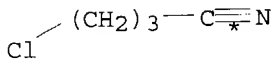


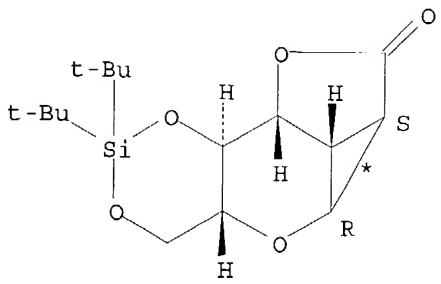
K
YIELD 79%

RX(4) RCT J **630-18-2**, B **361456-14-6**
RGT D 27607-77-8 Me3SiSO3CF3
PRO K **575444-69-8**
SOL 75-09-2 CH2Cl2

RX(5) OF 13 **L** + **B** ===> **M**

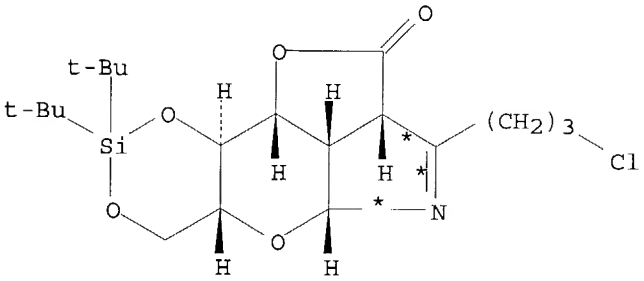


L



B

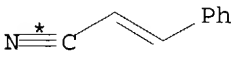
(5)



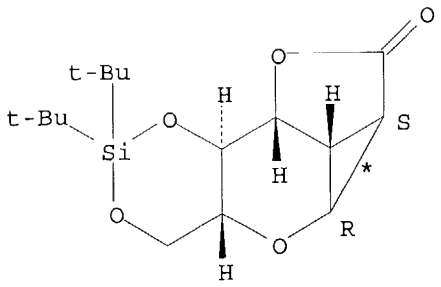
M
YIELD 87%

RX(5) RCT L **628-20-6**, B **361456-14-6**
RGT D 27607-77-8 Me3SiSO3CF3
PRO M **575444-70-1**
SOL 75-09-2 CH2Cl2

RX(6) OF 13 **N** + **B** ===> **O**



N



B

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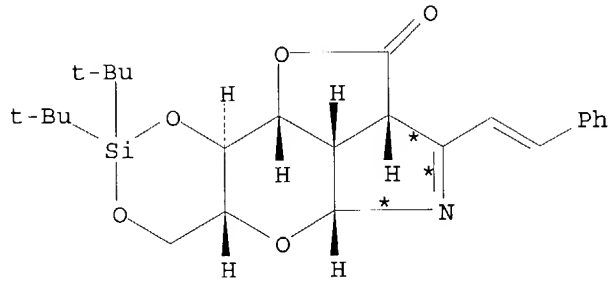
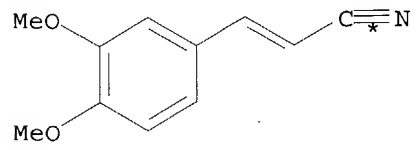


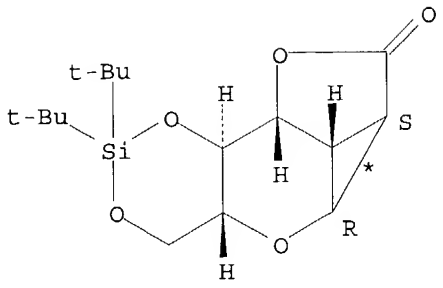
O
YIELD 60%

RX(6) RCT N **1885-38-7**, B **361456-14-6**
RGT D 27607-77-8 Me3SiSO3CF3
PRO O **575444-71-2**
SOL 75-52-5 MeNO2

RX(7) OF 13 **Q** + **B** ===> **R**



Q



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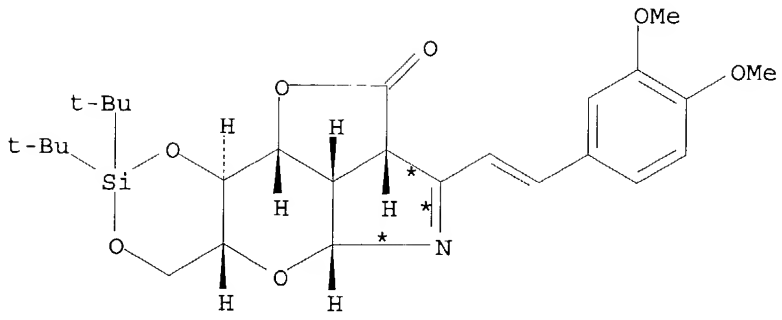
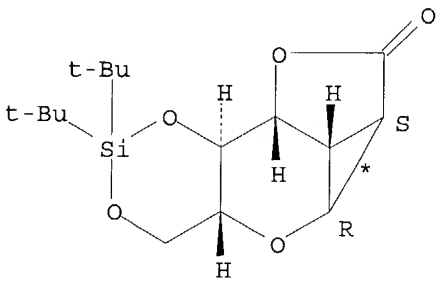


R
YIELD 75%

RX(7) RCT Q **37629-85-9**, B **361456-14-6**
RGT D 27607-77-8 Me3SiSO3CF3
PRO R **575444-72-3**
SOL 75-52-5 MeNO2

RX(8) OF 13 **S** + **B** ===> **T**

S



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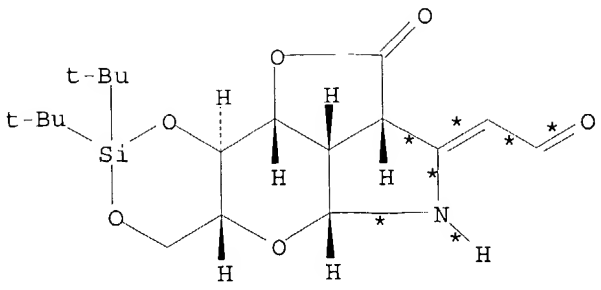
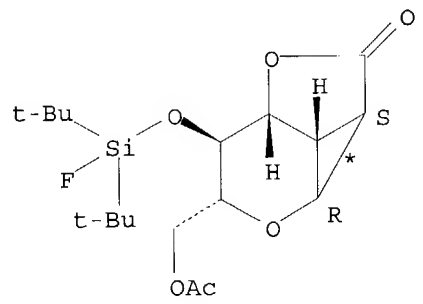


T
YIELD 78%

RX(8) RCT S **60838-50-8**, B **361456-14-6**
RGT D 27607-77-8 Me3SiSO3CF3
PRO T **575444-73-4**
SOL 75-09-2 CH2Cl2

RX(9) OF 13 **U** + **F** ===> **V**



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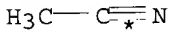
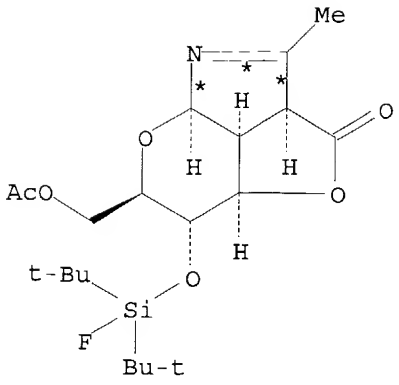


F

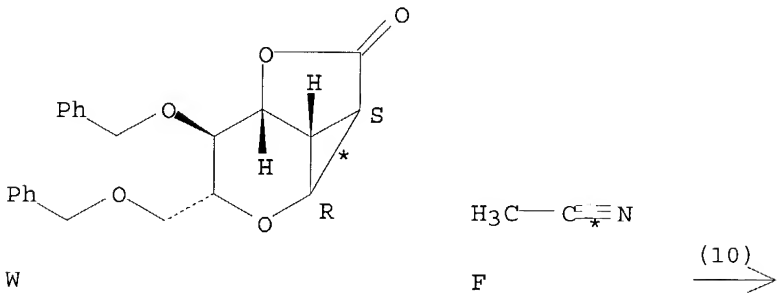
(9) →



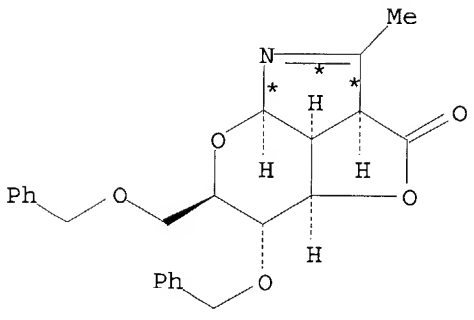
V
YIELD 92%

RX(9) RCT U **575444-74-5**, F **75-05-8**
RGT D 27607-77-8 Me3SiSO3CF3
PRO V **575444-77-8**
SOL 75-09-2 CH2Cl2

RX(10) OF 13 **W** + **F** ===> **X**



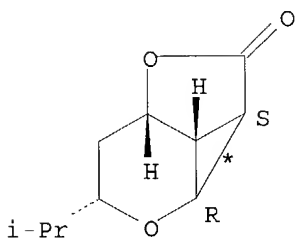
W F (10)



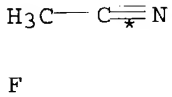
X
YIELD 90%

RX(10) RCT W **575444-75-6**, F **75-05-8**
RGT D 27607-77-8 Me3SiSO3CF3
PRO X **575444-78-9**
SOL 75-09-2 CH2Cl2

RX(11) OF 13 **Y** + **F** ===> **Z**



Y



F

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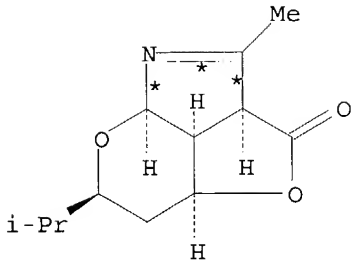
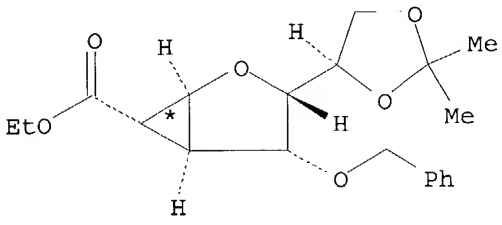


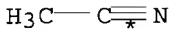
Z
YIELD 96%

RX(11) RCT Y **575444-76-7**, F **75-05-8**
RGT D 27607-77-8 Me3SiSO3CF3
PRO Z **575444-79-0**
SOL 75-09-2 CH2Cl2

RX(12) OF 13 **AA** + **F** ===> **AB**

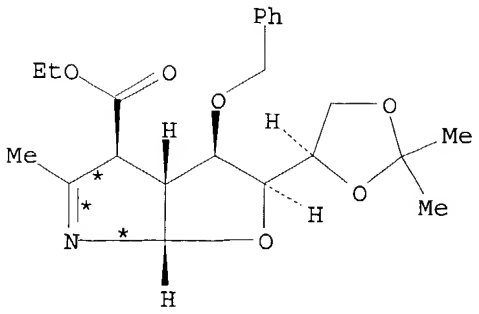


AA



F

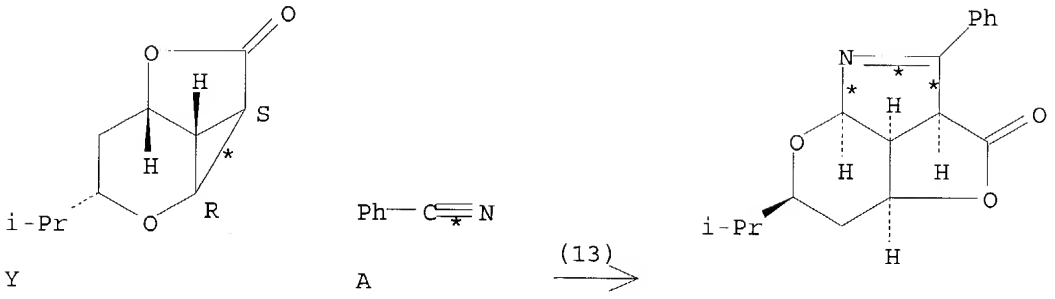
(12)



AB
YIELD 43%

RX(12) RCT AA **250369-61-0**, F **75-05-8**
RGT D 27607-77-8 Me3SiSO3CF3
PRO AB **575444-81-4**
SOL 75-09-2 CH2Cl2

RX(13) OF 13 **Y** + **A** ===> **AC**



Y A AC
YIELD 92%

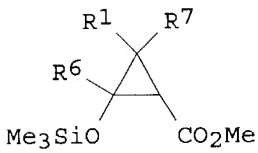
RX(13) RCT Y **575444-76-7**, A **100-47-0**
RGT D 27607-77-8 Me3SiSO3CF3
PRO AC **575444-80-3**
SOL 75-09-2 CH2Cl2

RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

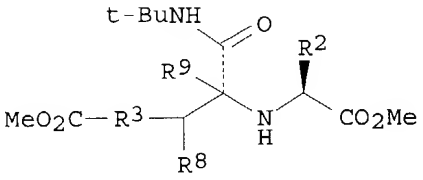
=> => d bib abs rx l33 tot

L33 ANSWER 1 OF 7 CASREACT COPYRIGHT 2004 ACS on STN
AN 136:6308 CASREACT
TI Siloxycyclopropanes in Ugi four-component reaction: a new method for the synthesis of highly substituted pyrrolidinone derivatives

AU Zimmer, Reinhold; Ziemer, Antje; Gruner, Margit; Brudgam, Irene; Hartl, Hans; Reissig, Hans-Ulrich
CS Institut fur Chemie - Organische Chemie, Freie Universitat Berlin, Berlin, 14195, Germany
SO Synthesis (**2001**), (11), 1649-1658
CODEN: SYNTBF; ISSN: 0039-7881
PB Georg Thieme Verlag
DT Journal
LA English
GI



I



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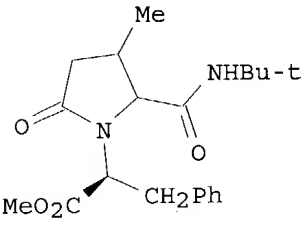
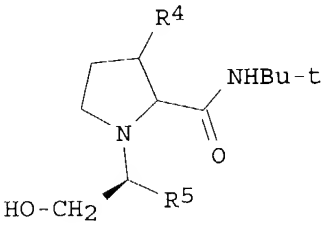


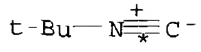
III



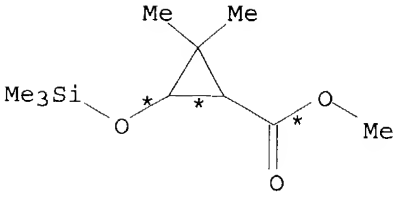
IV

AB Reaction of Me trimethylsiloxycyclopropanecarboxylates I (R1 = H, Me; R6 = H, Me; R7 = H, Me) with amino acids, tert-butylisonitrile and methanol furnished amino diacid derivs. II [R2 = Bn, CH2indolyl, Me, CHMeEt; R3 = CH2, (CH2)2; R8 = H, Me; R9 = H, Me] as the result of an Ugi 5-center 4-component reaction. This one-pot reaction involves .beta.-formyl esters such as MeOCOCH2CH(Me)COH as intermediate, which are liberated in situ. Adducts II could be thermally cyclized to provide .gamma.-lactams in good yields. The multi component reaction was combined with this cyclization process to a fairly efficient one-pot procedure. Thus, cyclopropane derivative I (R1 = H) was converted into .gamma.-lactam III in good yield. Two of the .gamma.-lactams were reduced with lithium aluminum hydride to give pyrrolidine derivs. IV (R4 = R5 = Me; R4 = H, R5 = Bn). Based on an X-ray anal. of the major diastereomer of compound IV (R4 = H, R5 = Bn), the diastereoselectivity of the 4-component reaction is discussed.

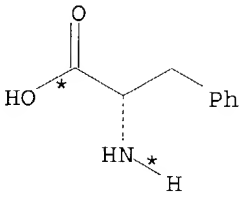
RX(17) OF 27 **A** + **AE** + C ===> **AF**



A

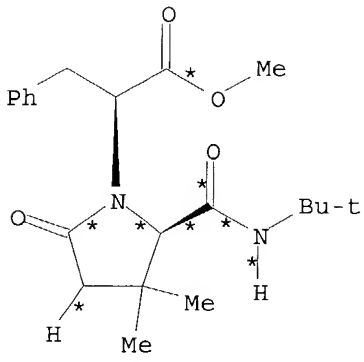


AE



C

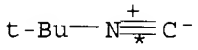
(17) ⟶



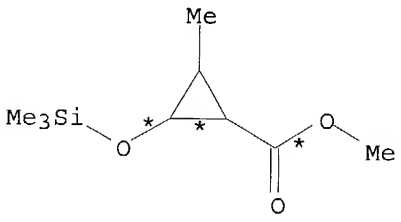
AF
YIELD 16%(53)

RX(17) RCT A **7188-38-7**, AE **77903-45-8**, C 63-91-2
PRO AF **374936-80-8**
SOL 67-56-1 MeOH

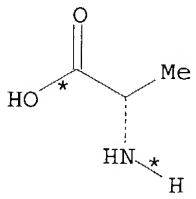
RX(20) OF 27 COMPOSED OF RX(4), RX(11)
RX(20) **A** + **J** + K + E ===> **U**



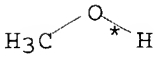
A



J

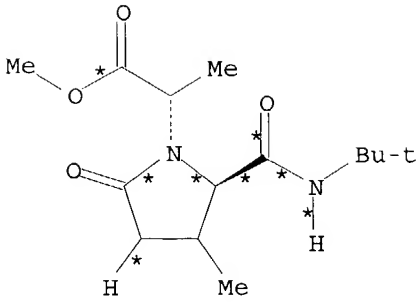


K



E

2 STEPS ⟶

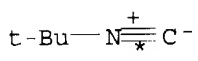


U
YIELD 71%(56)

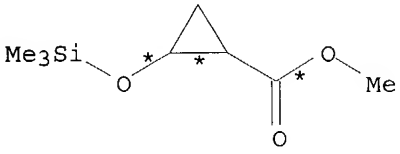
RX(4) RCT A **7188-38-7**, J **82884-40-0**, K 56-41-7, E 67-56-1
PRO L 374936-67-1
SOL 67-56-1 MeOH
NTE four Isomers 37:32:17:14 (R-major Isomer)

RX(11) RCT L 374936-67-1
PRO U **374936-74-0**
SOL 108-88-3 PhMe

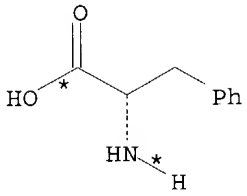
RX(21) OF 27 COMPOSED OF RX(5), RX(12)
RX(21) **A** + **M** + C + E ===> **V**



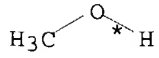
A



M

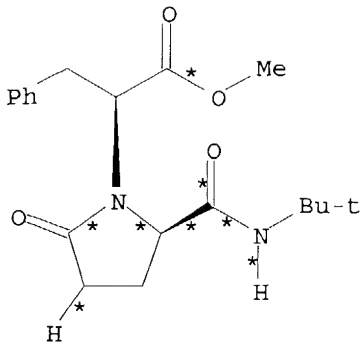


C



E

2 STEPS

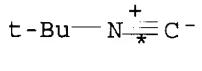


V
YIELD 96%(90)

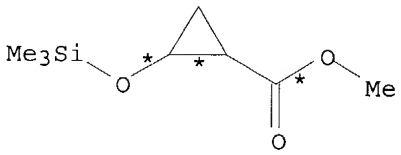
RX(5) RCT A **7188-38-7**, M **90288-79-2**, C 63-91-2, E 67-56-1
PRO N 374936-68-2
SOL 67-56-1 MeOH
NTE stereoselective

RX(12) RCT N 374936-68-2
PRO V **374936-75-1**
SOL 108-88-3 PhMe

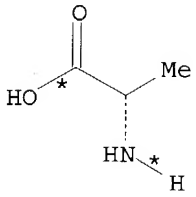
RX(22) OF 27 COMPOSED OF RX(6), RX(13)
RX(22) **A** + **M** + K + E ===> **W**



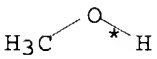
A



M

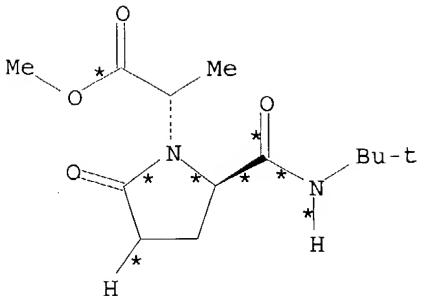


K



E

2 STEPS

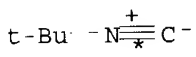


W
YIELD 86%(64)

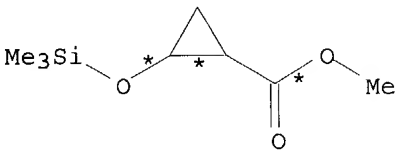
RX(6) RCT A **7188-38-7**, M **90288-79-2**, K 56-41-7, E 67-56-1
PRO O 374936-69-3
SOL 67-56-1 MeOH
NTE stereoselective

RX(13) RCT O 374936-69-3
PRO W **374936-76-2**
SOL 108-88-3 PhMe

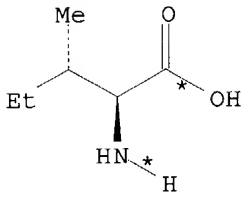
RX(23) OF 27 COMPOSED OF RX(7), RX(14)
RX(23) **A** + **M** + P + E ===> **X**



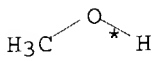
A



M

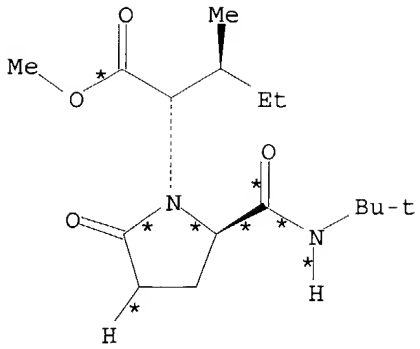


P



E

2 STEPS

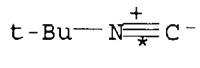


X
YIELD 82%(85)

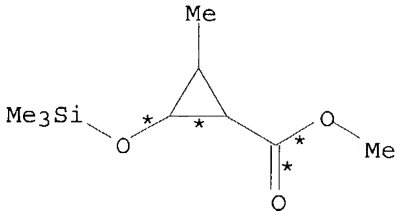
RX(7) RCT A **7188-38-7**, M **90288-79-2**, P 73-32-5, E 67-56-1
PRO Q 374936-70-6
SOL 67-56-1 MeOH
NTE stereoselective

RX(14) RCT Q 374936-70-6
PRO X **374936-77-3**
SOL 108-88-3 PhMe

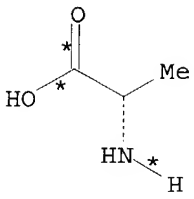
RX(26) OF 27 COMPOSED OF RX(4), RX(11), RX(16)
RX(26) **A** + **J** + K + E ===> **AD**



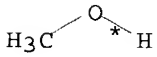
A



J

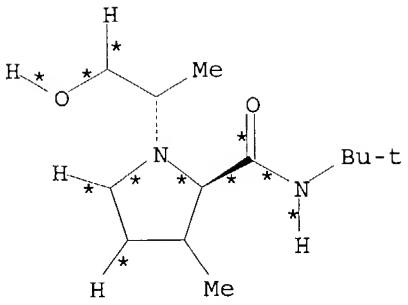


K



E

3 STEPS



AD
YIELD 16%

RX(4) RCT A **7188-38-7**, J **82884-40-0**, K 56-41-7, E 67-56-1
PRO L 374936-67-1
SOL 67-56-1 MeOH
NTE four Isomers 37:32:17:14 (R-major Isomer)

RX(11) RCT L 374936-67-1
PRO U 374936-74-0
SOL 108-88-3 PhMe

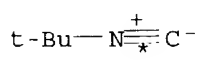
RX(16) RCT U 374936-74-0

STAGE(1)
RGT Z 16853-85-3 LiAlH4
SOL 109-99-9 THF

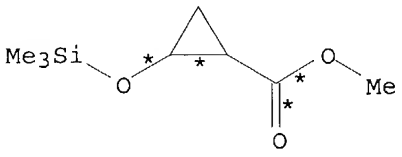
STAGE(2)
RGT AA 7732-18-5 Water

STAGE(3)
RGT AB 1310-73-2 NaOH
SOL 7732-18-5 Water
PRO AD **374936-79-5**

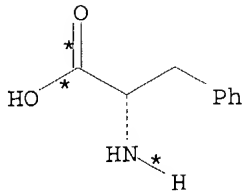
RX(27) OF 27 COMPOSED OF RX(5), RX(12), RX(15)
RX(27) **A** + **M** + C + E ===> **Y**



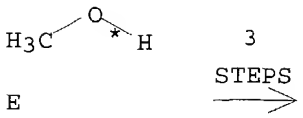
A



M

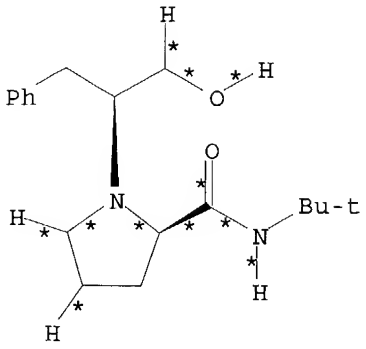


C



E

3
STEPS



Y
YIELD 81%

RX(5) RCT A **7188-38-7**, M **90288-79-2**, C 63-91-2, E 67-56-1
PRO N 374936-68-2
SOL 67-56-1 MeOH
NTE stereoselective

RX(12) RCT N 374936-68-2
PRO V 374936-75-1
SOL 108-88-3 PhMe

RX(15) RCT V 374936-75-1

STAGE(1)
RGT Z 16853-85-3 LiAlH4
SOL 109-99-9 THF

STAGE(2)
RGT AA 7732-18-5 Water

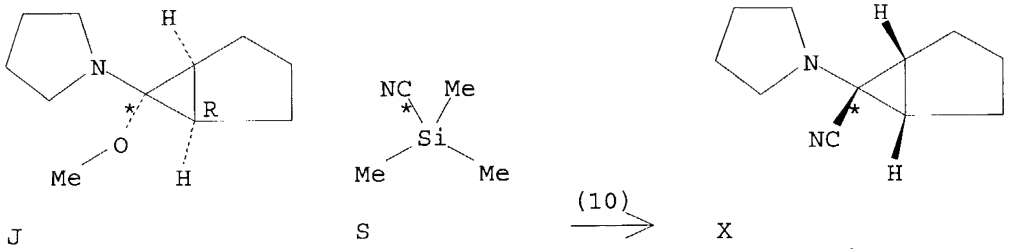
STAGE(3)
RGT AB 1310-73-2 NaOH
SOL 7732-18-5 Water
PRO Y **374936-78-4**

RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 2 OF 7 CASREACT COPYRIGHT 2004 ACS on STN
AN 130:311547 CASREACT
TI Ring-Fused Cyclopropanone N,O-Acetals. Electrochemical Preparation and Their Reactivities under Acidic Conditions

AU Chiba, Toshiro; Saitoh, Isao; Okimoto, Mitsuhiro; Tanase, Tomokazu; Yano, Sigenobu
CS Department of Applied Chemistry, Kitami Institute of Technology, Kitami, 090, Japan
SO Journal of Organic Chemistry **(1999)**, 64(7), 2516-2519
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
AB The electrochem. reaction of cyclic enamines gave fused N,O-cyclopropanone acetals. The cyanation of the latter gave the corresponding amino nitriles. For example, the electrochem. reaction of N,N-diethyl-1-cyclohexen-1-amine gave 6-endo-(dimethylamino)-6-exo-methoxybicyclo[3.1.0]hexane. Further cyanation of the latter with trimethylsilyl cyanide and boron trifluoride-etherate gave 6-exo-cyano-6-endo-(diethylamino)bicyclo[3.1.0]hexane.

RX(10) OF 32 ...J + S ===> X



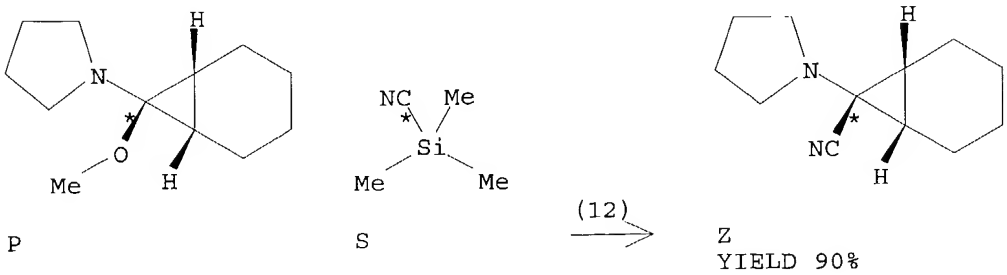
J S X
YIELD 63%

RX(10) RCT J **223482-73-3**, S **7677-24-9**

STAGE(1)
RGT U 109-63-7 BF3-Et2O
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT F 7732-18-5 Water
PRO X **214780-98-0**

RX(12) OF 32 ...P + S ===> Z



P S Z
YIELD 90%

RX(12) RCT P **223482-87-9**, S **7677-24-9**

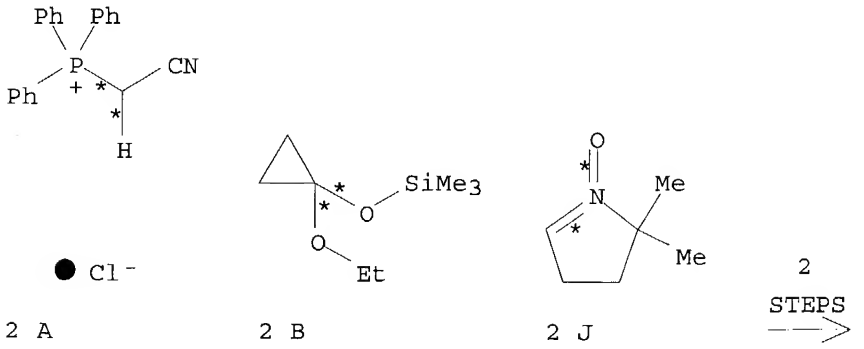
STAGE(1)
RGT U 109-63-7 BF3-Et2O
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT F 7732-18-5 Water
PRO Z **76826-53-4**

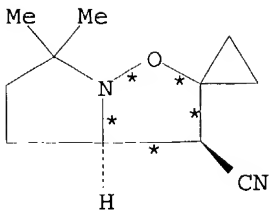
RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 3 OF 7 CASREACT COPYRIGHT 2004 ACS on STN
AN 129:289743 CASREACT
TI Cyanomethylene cyclopropane, a useful dipolarophile and dienophile in [2+3] and [2+4] cycloadditions
AU Mauduit, Marc; Kouklovsky, Cyrille; Langlois, Yves
CS Laboratoire de Synthese des Substances Naturelles Associe au CNRS, ICMO, Universite de Paris-sud, Orsay, 91405, Fr.
SO Tetrahedron Letters (**1998**), 39(38), 6857-6860
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
AB Cyanomethylene cyclopropane, prepared for the first time on large scale, proved to be a reactive dipolarophile and dienophile in several cycloaddns. The reactivity of this compound has been compared with 3-methyl-2-butenenitrile, Et 3-methyl-2-butenoate, and ethoxycarbonylmethylene cyclopropane.

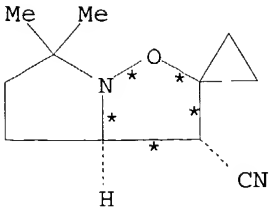
RX(12) OF 16 COMPOSED OF RX(1), RX(2)
RX(12) 2 **A** + 2 **B** + 2 J ===> **K** + L



2 A 2 B 2 J



K
YIELD 87%(80)



L
YIELD 87%(20)

RX(1) RCT A **4336-70-3**

STAGE(1)
RGT D 1310-73-2 NaOH
SOL 64-17-5 EtOH

STAGE(2)
RCT B **27374-25-0**
RGT E 75-77-4 Me3SiCl
SOL 67-56-1 MeOH

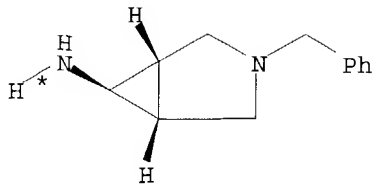
STAGE(3)
RGT F 65-85-0 BzOH
SOL 71-43-2 Benzene
PRO C 214262-61-0
NTE CONVERGENT PREPN.

RX(2) RCT C 214262-61-0, J 3317-61-1
PRO K **214262-62-1**, L 214262-63-2
SOL 108-88-3 PhMe
NTE STEREOSELECTIVE

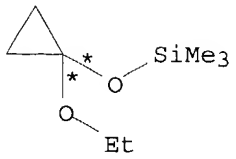
RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 4 OF 7 CASREACT COPYRIGHT 2004 ACS on STN
AN 124:86390 CASREACT
TI A simple method for the formation of cyclopropylamines: the first synthesis of tricyclopropylamine.
AU Gillaspy, Melissa; Lefker, Bruce A.; Hada, William A.; Hoover, Dennis J.
CS Pfizer Central Res., Groton, CT, 06340, USA
SO Tetrahedron Letters (**1995**), 36(41), 7399-402
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier
DT Journal
LA English
AB Treatment of a variety of secondary and primary amines with [(1-ethoxycyclopropyl)oxy]trimethylsilane and NaBH3CN in MeOH gave mono- and dicyclopropylamines in 41-91% yield. Sterically hindered di- and tricyclopropylamines, including tricyclopropylamine, were prepared The pKas of some mono-, di- and tricyclopropylamines were measured showing a reduction of .apprx.1-2 pKa unit per added cyclopropyl group.

RX(2) OF 8 G + 2 **B** ===> **H**

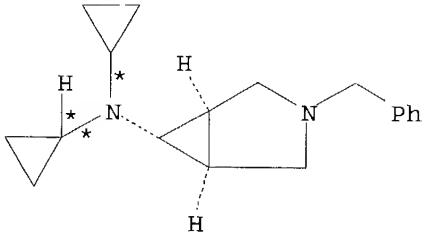


G



2 B

(2)

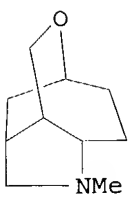


● HCl

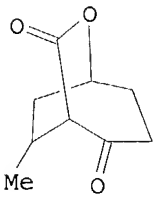
H
YIELD 66%

RX(2) RCT G 151860-17-2, B **27374-25-0**
RGT D 64-19-7 AcOH, E **25895-60-7** NaBH3CN
PRO H **172537-66-5**
SOL 67-56-1 MeOH
NTE reflux overnight

L33 ANSWER 5 OF 7 CASREACT COPYRIGHT 2004 ACS on STN
AN 113:78789 CASREACT
TI A synthetic approach to gelsemicine
AU Hamer, Neil K.
CS Univ. Chem. Lab., Cambridge, CB2 1EW, UK
SO Journal of the Chemical Society, Chemical Communications (**1990**), (2), 102-3
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
GI



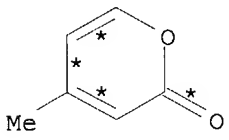
I



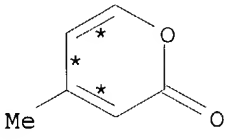
II

AB The oxaazatricycloundecane ring I present in gelsemicine was prepared from the cycloadduct of 3,3-dimethoxycyclopropene and 4-methyl-2H-pyran-2-one via the oxabicyclononanedione II. The structure of II was detd by x-ray crystallog.

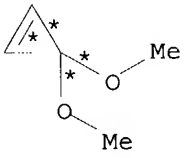
RX(29) OF 29 COMPOSED OF RX(8), RX(1), RX(2), RX(3), RX(7), RX(4)
RX(29) 2 Z + 2 **AA** + 2 W ===> **N**



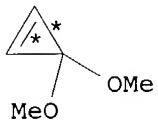
Z



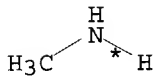
Z



AA

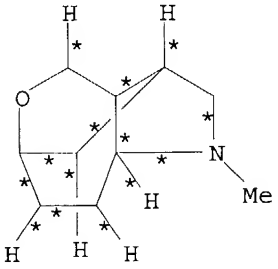


AA



2 W

6 STEPS



N
YIELD 82%

RX(8) RCT Z 22682-12-8, AA **23529-83-1**
PRO A 128562-30-1

RX(1) RCT A 128562-30-1
RGT C 1333-74-0 H2
PRO B 128562-31-2
CAT 7440-16-6 Rh

RX(2) RCT B 128562-31-2

STAGE(1)
RGT F 16853-85-3 LiAlH4

STAGE(2)
RGT G 98-59-9 TsCl, H 7646-69-7 NaH
PRO E 128562-32-3

RX(3) RCT E 128562-32-3
RGT J 7647-01-0 HCl
PRO I 128562-35-6
SOL 67-56-1 MeOH, 7732-18-5 Water

RX(7) RCT W 74-89-5, I 128562-35-6
RGT Y **25895-60-7** NaBH3CN
PRO M 128656-99-5, X 128561-71-7
NTE 84% overall

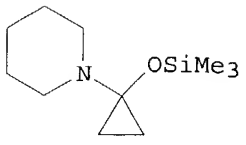
RX(4) RCT M 128656-99-5

STAGE(1)
RGT O 7681-52-9 NaOCl

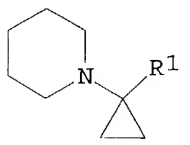
STAGE(2)
RGT P 76-05-1 F3CCO2H

STAGE(3)
RGT Q 1310-58-3 KOH
SOL 67-56-1 MeOH
PRO N **128562-29-8**

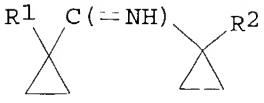
L33 ANSWER 6 OF 7 CASREACT COPYRIGHT 2004 ACS on STN
AN 112:35605 CASREACT
TI Cyclopropanone equivalents from 3-chloropropionic acid. Use of 1-piperidino-1-trimethylsilyloxycyclopropane in synthetic applications
AU Wasserman, Harry H.; Dion, Robert P.; Fukuyama, James
CS Dep. Chem., Yale Univ., New Haven, CT, 06511, USA
SO Tetrahedron (**1989**), 45(10), 3203-16
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
GI



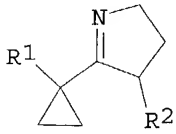
I



II



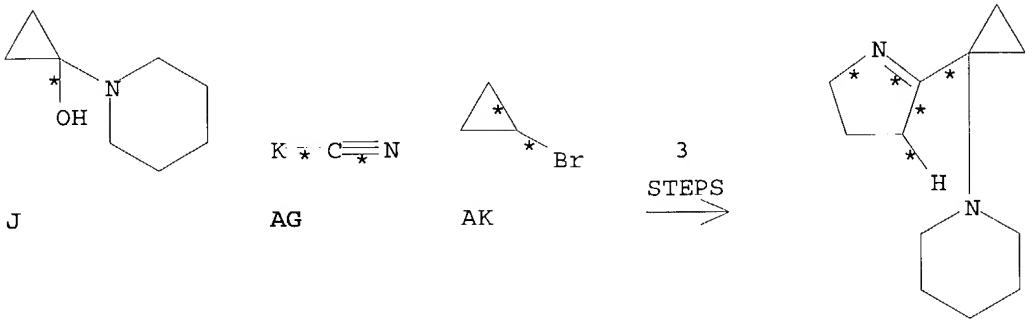
III



IV

AB 3-Chloropropionic acid piperidide was treated with Na and Me3SiCl to give cyclopropane I; the treatment of I with Grignard reagents gave II (R1 = vinyl, cyclopentenyl, Ph, Et). Cyclopropanecarbonitriles underwent an addition reaction with cyclopropyllithium compds. to give ketimines III (R1 = piperidino, H; R2 = H, SPh), which rearranged to pyrrolines IV. The rearrangement of III (R1 = H, R2 = SPh) gave IV (R1 = SPh, R2 = H) in addition to IV (R1 = H, R2 = SPh).

RX(62) OF 88 COMPOSED OF RX(12), RX(13), RX(14)
RX(62) **J** + **AG** + AK ===> **AO**



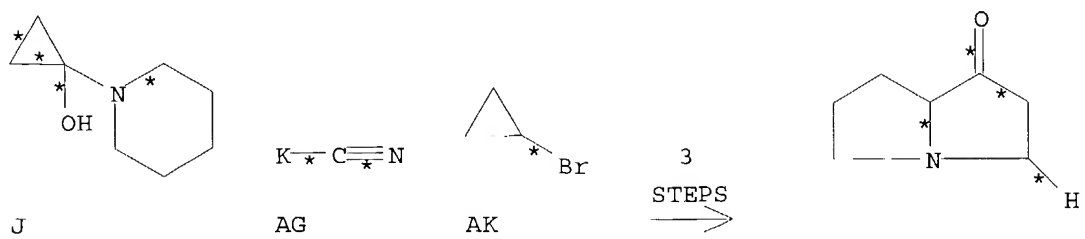
J **AG** AK **AO**
YIELD 77%

RX(12) RCT J **27161-21-3**, AG **151-50-8**
RGT AI 64-19-7 AcOH
PRO AH 82479-58-1
SOL 7732-18-5 Water

RX(13) RCT AH 82479-58-1, AK 4333-56-6
RGT AM 109-72-8 BuLi
PRO AL 82479-59-2
SOL 109-66-0 Pentane, 60-29-7 Et2O

RX(14) RCT AL 82479-59-2
PRO AO **82479-60-5**
SOL 106-42-3 1,4-Xylene

RX(63) OF 88 COMPOSED OF RX(12), RX(13), RX(15)
RX(63) **J** + **AG** + AK ===> **AQ**



J AG AK AQ
YIELD 32%

RX(12) RCT J **27161-21-3**, AG **151-50-8**
RGT AI 64-19-7 AcOH
PRO AH 82479-58-1
SOL 7732-18-5 Water

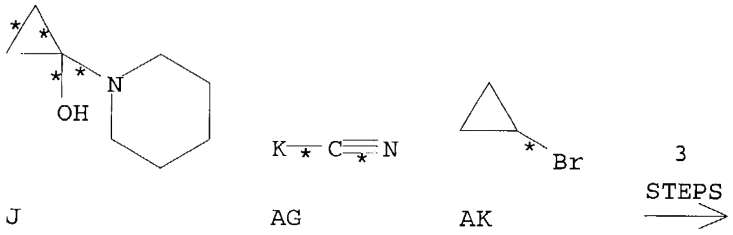
RX(13) RCT AH 82479-58-1, AK 4333-56-6
RGT AM 109-72-8 BuLi
PRO AL 82479-59-2
SOL 109-66-0 Pentane, 60-29-7 Et2O

RX(15) RCT AL 82479-59-2

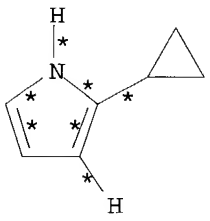
STAGE(1)
RGT AR 10035-10-6 HBr
SOL 60-29-7 Et2O

STAGE(2)
RGT AS 7647-01-0 HCl
SOL 7732-18-5 Water
PRO AQ **14174-83-5**
NTE 2nd step pyrolysis

RX(64) OF 88 COMPOSED OF RX(12), RX(13), RX(21)
RX(64) **J** + **AG** + AK ===> **BE**



J AG AK



BE
YIELD 31%

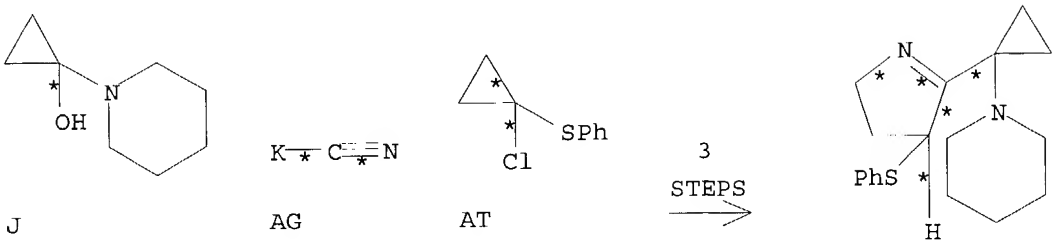
RX(12) RCT J **27161-21-3**, AG **151-50-8**
RGT AI 64-19-7 AcOH
PRO AH 82479-58-1
SOL 7732-18-5 Water

RX(13) RCT AH 82479-58-1, AK 4333-56-6
RGT AM 109-72-8 BuLi

PRO AL 82479-59-2
SOL 109-66-0 Pentane, 60-29-7 Et2O

RX(21) RCT AL 82479-59-2
RGT BF 353-42-4 Me2O.BF3
PRO BE **87385-10-2**
SOL 1330-20-7 Xylene

RX(65) OF 88 COMPOSED OF RX(12), RX(17), RX(19)
RX(65) **J** + **AG** + AT ===> **AZ**



J AG AT

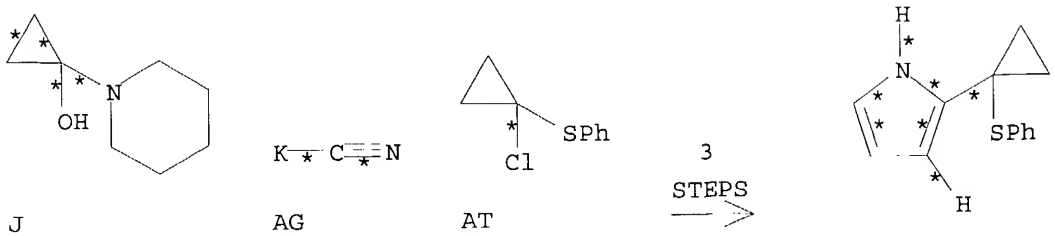
AZ
YIELD 69%

RX(12) RCT J **27161-21-3**, AG **151-50-8**
RGT AI 64-19-7 AcOH
PRO AH 82479-58-1
SOL 7732-18-5 Water

RX(17) RCT AH 82479-58-1, AT 64416-57-5
RGT AM 109-72-8 BuLi
PRO AU 87385-05-5
SOL 109-99-9 THF, 110-54-3 Hexane

RX(19) RCT AU 87385-05-5
RGT BA 12125-02-9 NH4Cl
PRO AZ **87385-07-7**
SOL 106-42-3 1,4-Xylene

RX(66) OF 88 COMPOSED OF RX(12), RX(17), RX(22)
RX(66) **J** + **AG** + AT ===> **BG**



J AG AT

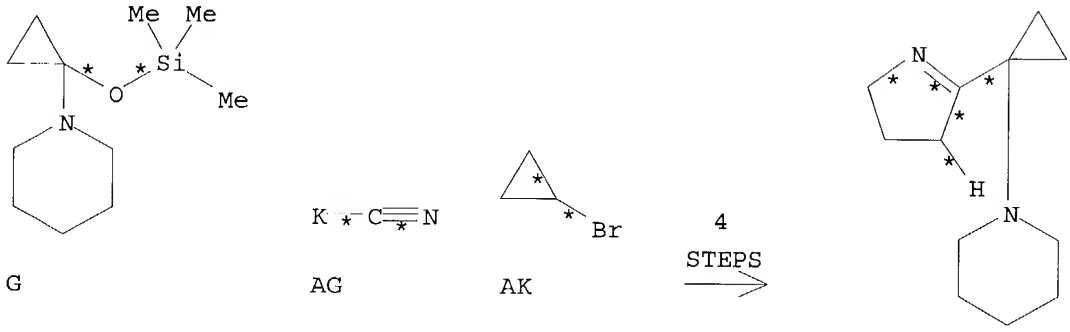
BG
YIELD 42%

RX(12) RCT J **27161-21-3**, AG **151-50-8**
RGT AI 64-19-7 AcOH
PRO AH 82479-58-1
SOL 7732-18-5 Water

RX(17) RCT AH 82479-58-1, AT 64416-57-5
RGT AM 109-72-8 BuLi
PRO AU 87385-05-5
SOL 109-99-9 THF, 110-54-3 Hexane

RX(22) RCT AU 87385-05-5
RGT BF 353-42-4 Me2O.BF3
PRO BG **87385-11-3**
SOL 109-99-9 THF

RX(67) OF 88 COMPOSED OF RX(3), RX(12), RX(13), RX(14)
RX(67) **G** + **AG** + AK ===> **AO**



G AG AK

AO
YIELD 77%

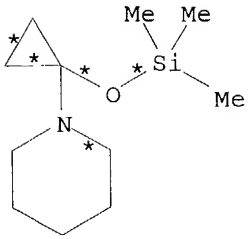
RX(3) RCT G **82125-98-2**
RGT K 429-41-4 Bu4N.F
PRO J 27161-21-3
SOL 67-56-1 MeOH

RX(12) RCT J 27161-21-3, AG **151-50-8**
RGT AI 64-19-7 AcOH
PRO AH 82479-58-1
SOL 7732-18-5 Water

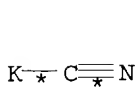
RX(13) RCT AH 82479-58-1, AK 4333-56-6
RGT AM 109-72-8 BuLi
PRO AL 82479-59-2
SOL 109-66-0 Pentane, 60-29-7 Et2O

RX(14) RCT AL 82479-59-2
PRO AO **82479-60-5**
SOL 106-42-3 1,4-Xylene

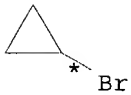
RX(68) OF 88 COMPOSED OF RX(3), RX(12), RX(13), RX(15)
RX(68) **G** + **AG** + AK ===> **AQ**



G

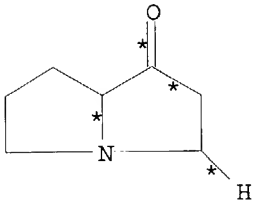


AG



AK

4 STEPS



AQ
YIELD 32%

RX(3) RCT G **82125-98-2**
RGT K 429-41-4 Bu4N.F
PRO J 27161-21-3
SOL 67-56-1 MeOH

RX(12) RCT J 27161-21-3, AG **151-50-8**
RGT AI 64-19-7 AcOH
PRO AH 82479-58-1
SOL 7732-18-5 Water

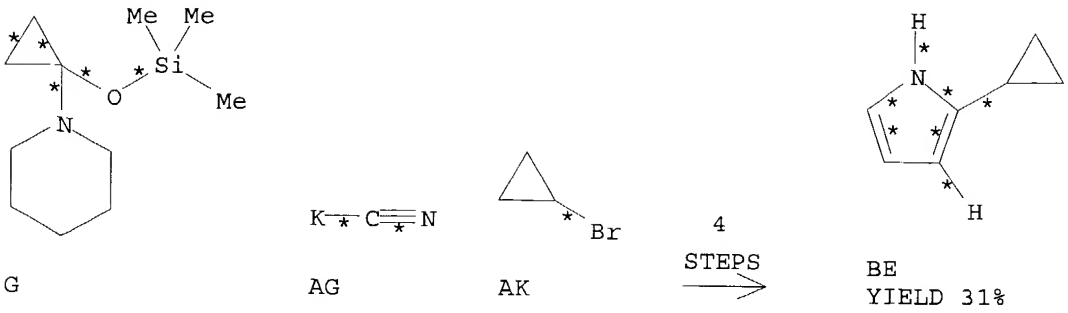
RX(13) RCT AH 82479-58-1, AK 4333-56-6
RGT AM 109-72-8 BuLi
PRO AL 82479-59-2
SOL 109-66-0 Pentane, 60-29-7 Et2O

RX(15) RCT AL 82479-59-2

STAGE(1)
RGT AR 10035-10-6 HBr
SOL 60-29-7 Et2O

STAGE(2)
RGT AS 7647-01-0 HCl
SOL 7732-18-5 Water
PRO AQ **14174-83-5**
NTE 2nd step pyrolysis

RX(69) OF 88 COMPOSED OF RX(3), RX(12), RX(13), RX(21)
RX(69) **G** + **AG** + AK ===> **BE**



G AG AK BE
YIELD 31%

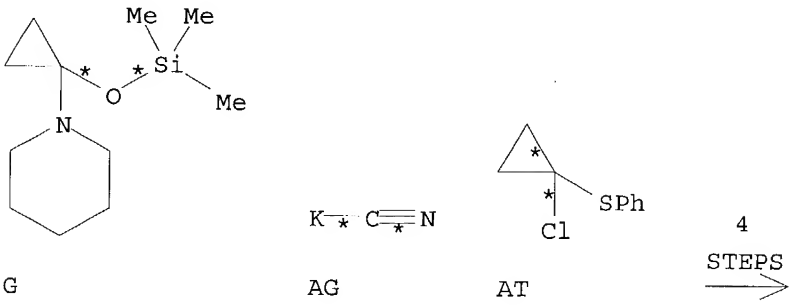
RX(3) RCT G **82125-98-2**
RGT K 429-41-4 Bu4N.F
PRO J 27161-21-3
SOL 67-56-1 MeOH

RX(12) RCT J 27161-21-3, AG **151-50-8**
RGT AI 64-19-7 AcOH
PRO AH 82479-58-1
SOL 7732-18-5 Water

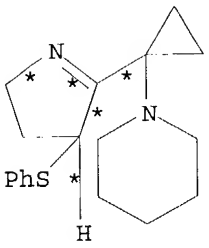
RX(13) RCT AH 82479-58-1, AK 4333-56-6
RGT AM 109-72-8 BuLi
PRO AL 82479-59-2
SOL 109-66-0 Pentane, 60-29-7 Et2O

RX(21) RCT AL 82479-59-2
RGT BF 353-42-4 Me2O.BF3
PRO BE **87385-10-2**
SOL 1330-20-7 Xylene

RX(70) OF 88 COMPOSED OF RX(3), RX(12), RX(17), RX(19)
RX(70) **G** + **AG** + AT ===> **AZ**



G AG AT



AZ
YIELD 69%

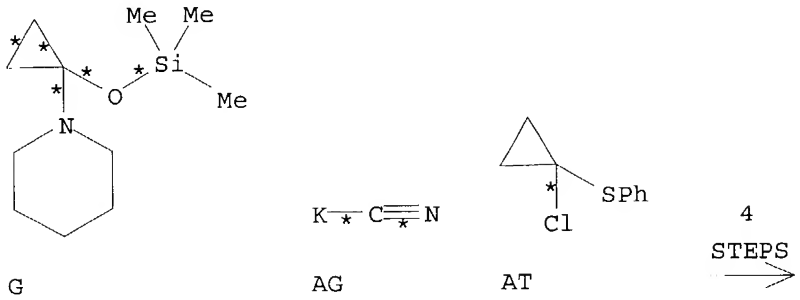
RX(3) RCT G **82125-98-2**
RGT K 429-41-4 Bu4N.F
PRO J 27161-21-3
SOL 67-56-1 MeOH

RX(12) RCT J 27161-21-3, AG **151-50-8**
RGT AI 64-19-7 AcOH
PRO AH 82479-58-1
SOL 7732-18-5 Water

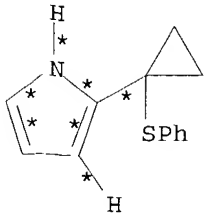
RX(17) RCT AH 82479-58-1, AT 64416-57-5
RGT AM 109-72-8 BuLi
PRO AU 87385-05-5
SOL 109-99-9 THF, 110-54-3 Hexane

RX(19) RCT AU 87385-05-5
RGT BA 12125-02-9 NH4Cl
PRO AZ **87385-07-7**
SOL 106-42-3 1,4-Xylene

RX(71) OF 88 COMPOSED OF RX(3), RX(12), RX(17), RX(22)
RX(71) **G** + **AG** + AT ===> **BG**



G AG AT 4 STEPS



BG
YIELD 42%

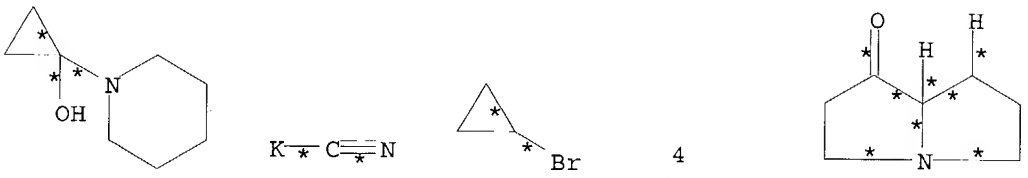
RX(3) RCT G **82125-98-2**
RGT K 429-41-4 Bu4N.F
PRO J 27161-21-3
SOL 67-56-1 MeOH

RX(12) RCT J 27161-21-3, AG **151-50-8**
RGT AI 64-19-7 AcOH
PRO AH 82479-58-1
SOL 7732-18-5 Water

RX(17) RCT AH 82479-58-1, AT 64416-57-5
RGT AM 109-72-8 BuLi
PRO AU 87385-05-5
SOL 109-99-9 THF, 110-54-3 Hexane

RX(22) RCT AU 87385-05-5
RGT BF 353-42-4 Me2O.BF3
PRO BG **87385-11-3**
SOL 109-99-9 THF

RX(73) OF 88 COMPOSED OF RX(12), RX(13), RX(14), RX(16)
RX(73) **J** + **AG** + AK ===> **AQ**



J AG AK 4 STEPS AQ
YIELD 51%

RX(12) RCT J **27161-21-3**, AG **151-50-8**
RGT AI 64-19-7 AcOH
PRO AH 82479-58-1
SOL 7732-18-5 Water

RX(13) RCT AH 82479-58-1, AK 4333-56-6
RGT AM 109-72-8 BuLi
PRO AL 82479-59-2
SOL 109-66-0 Pentane, 60-29-7 Et2O

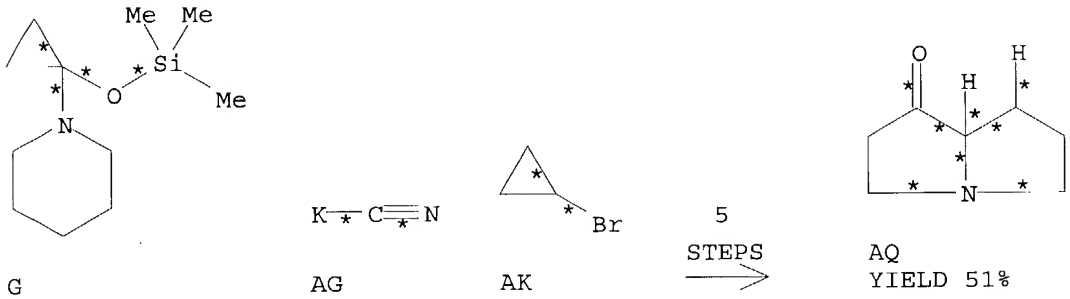
RX(14) RCT AL 82479-59-2
PRO AO 82479-60-5
SOL 106-42-3 1,4-Xylene

RX(16) RCT AO 82479-60-5

STAGE(1)
RGT AR 10035-10-6 HBr
SOL 60-29-7 Et2O

STAGE(2)
RGT AS 7647-01-0 HCl
SOL 7732-18-5 Water
PRO AQ **14174-83-5**
NTE 2nd step pyrolysis

RX(86) OF 88 COMPOSED OF RX(3), RX(12), RX(13), RX(14), RX(16)
RX(86) **G** + **AG** + AK ===> **AQ**



G AG AK AQ
YIELD 51%

RX(3) RCT G **82125-98-2**
RGT K 429-41-4 Bu4N.F
PRO J 27161-21-3
SOL 67-56-1 MeOH

RX(12) RCT J 27161-21-3, AG **151-50-8**
RGT AI 64-19-7 AcOH
PRO AH 82479-58-1
SOL 7732-18-5 Water

RX(13) RCT AH 82479-58-1, AK 4333-56-6
RGT AM 109-72-8 BuLi
PRO AL 82479-59-2
SOL 109-66-0 Pentane, 60-29-7 Et2O

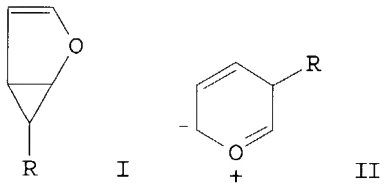
RX(14) RCT AL 82479-59-2
PRO AO 82479-60-5
SOL 106-42-3 1,4-Xylene

RX(16) RCT AO 82479-60-5

STAGE(1)
RGT AR 10035-10-6 HBr
SOL 60-29-7 Et2O

STAGE(2)
RGT AS 7647-01-0 HCl
SOL 7732-18-5 Water
PRO AQ **14174-83-5**
NTE 2nd step pyrolysis

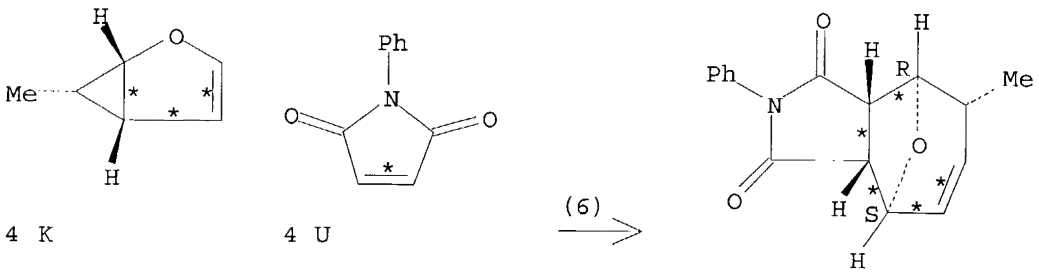
L33 ANSWER 7 OF 7 CASREACT COPYRIGHT 2004 ACS on STN
AN 110:74558 CASREACT
TI Organic reactions at high pressure: the mechanism of the homo-Diels-Alder reaction of homofuran (2-oxabicyclo[3.1.0]hex-3-ene)
AU Klaerner, Frank Gerrit; Schroer, Dietmar
CS Fak. Chem., Univ. Bochum, Bochum, D-4630/1, Fed. Rep. Ger.
SO Chemische Berichte (**1989**), 122(1), 179-85
CODEN: CHBEAM; ISSN: 0009-2940
DT Journal
LA German
GI



I II

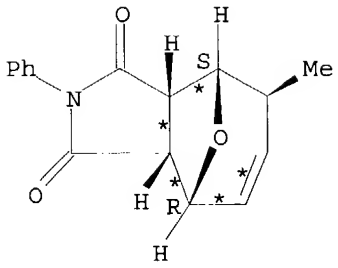
AB High pressure kinetics of the title reaction of (-)-I (R = H) with trans-NCCH:CHCN, to give the optically active adduct supports a [(.pi.2 + .sigma.2) + .pi.2] cycloaddn. mechanism which does not involve ring opening to the dihydropyrilium zwitterion II; II is involved in the racemization of (-)-I (R = H). The reaction of I (R = .alpha.-Me, .beta.-Me) shows that the cycloaddn. proceeds exo with respect to the three-membered ring.

RX(6) OF 71 ...4 **K** + 4 **U** ===> **V** + W + X + Y

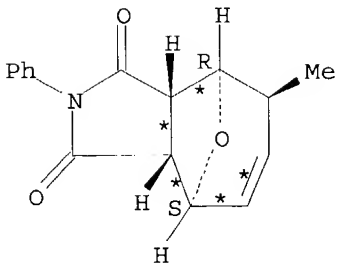


4 K 4 U (6) V

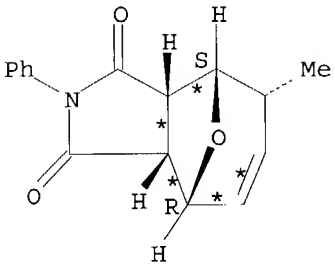
YIELD 50%



W
YIELD 40%



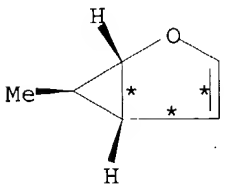
X



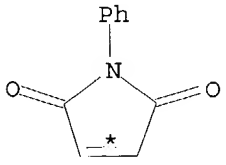
Y

RX(6) RCT K **42311-33-1**, U 941-69-5
RGT Z **117065-57-3** 8-Oxabicyclo[3.2.1]oct-2-ene-6,7-dicarbonitrile, (exo,exo)-
PRO V **116997-00-3**, W 117065-63-1, X 117065-64-2, Y 117065-65-3
SOL 666-52-4 Acetone-d6

RX(21) OF 71 COMPOSED OF RX(11), RX(6)
RX(21) 4 **L** + 4 U ===> **V** + W + X + Y

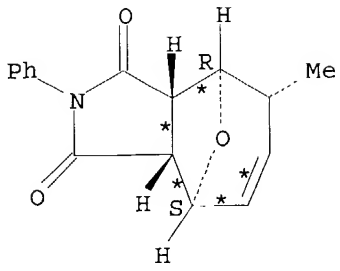


4 L

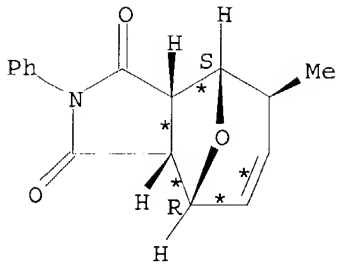


4 U

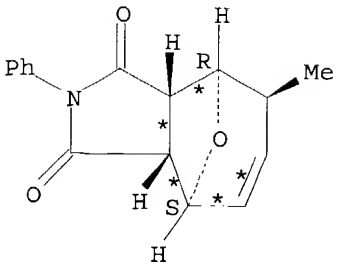
2 STEPS



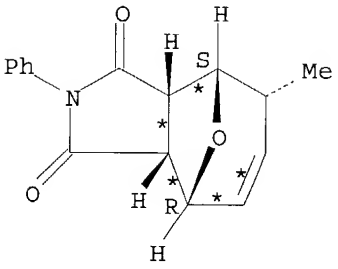
V
YIELD 50%



W
YIELD 40%



X



Y

RX(11) RCT L **42204-89-7**
PRO K 42311-33-1
SOL 110-00-9 Furan
NTE 80.degree.

RX(6) RCT K 42311-33-1, U 941-69-5
RGT Z **117065-57-3** 8-Oxabicyclo[3.2.1]oct-2-ene-6,7-dicarbonitrile, (exo,exo)-
PRO V **116997-00-3**, W 117065-63-1, X 117065-64-2, Y 117065-65-3
SOL 666-52-4 Acetone-d6

=> b reg
FILE 'REGISTRY' ENTERED AT 10:48:42 ON 14 JUL 2004

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 13 JUL 2004 HIGHEST RN 709042-93-3
DICTIONARY FILE UPDATES: 13 JUL 2004 HIGHEST RN 709042-93-3

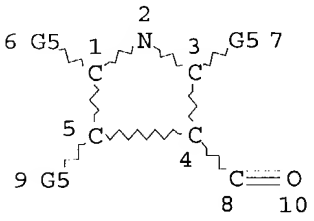
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d que stat l46
L3 STR



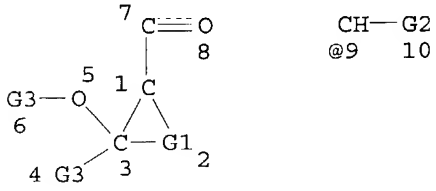
VAR G5=H/CY/AK
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 5
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
L46 36074 SEA FILE=REGISTRY SSS FUL L3

100.0% PROCESSED 162043 ITERATIONS 36074 ANSWERS
SEARCH TIME: 00.00.08

=> d que stat l47
L1 STR



VAR G1=CH2/9
VAR G2=CY/AK
VAR G3=H/AK/CY
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
L47 679 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 3326 ITERATIONS 679 ANSWERS
SEARCH TIME: 00.00.01

=> b hcap
FILE 'HCAPLUS' ENTERED AT 10:44:59 ON 14 JUL 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 14 Jul 2004 VOL 141 ISS 3
FILE LAST UPDATED: 13 Jul 2004 (20040713/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> b hcap
FILE 'HCAPLUS' ENTERED AT 11:06:45 ON 14 JUL 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

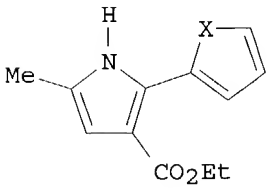
FILE COVERS 1907 - 14 Jul 2004 VOL 141 ISS 3
FILE LAST UPDATED: 13 Jul 2004 (20040713/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

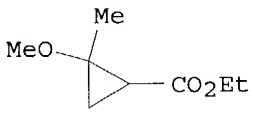
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d bib abs fhitstr hitrn l57 tot

L57 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2004:141810 HCAPLUS
DN 140:339152
TI Synthesis of 2,2'-bipyrroles and 2,2'-thienylpyrroles from donor-acceptor cyclopropanes and 2-cyanoheteroles
AU **Yu, Ming**; Pantos, G. Dan; Sessler, Jonathan L.; **Pagenkopf, Brian L.**
CS Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX, 78712, USA
SO Organic Letters (2004), 6(6), 1057-1059
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
GI



I

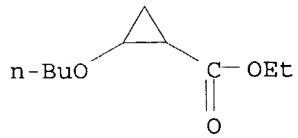


II

AB Two series of 2,2'-bipyrroles, e.g., I (X = NH), and 2,2'-thienylpyrroles, e.g., I (X = S), have been prepared by trimethylsilyl trifluoromethanesulfonate-mediated reaction of donor-acceptor cyclopropanes, e.g., II, with 2-cyanopyrroles and 2-cyanothiophene, resp. This method opened the door for synthesis of a wide variety of unsym. bipyrroles and thienylpyrroles.

IT **78932-45-3**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**;
PREP (Preparation)
(preparation of bipyrrolecarboxylates and thienylpyrrolecarboxylates via heterocyclization of alkoxycyclopropanecarboxylates with cyanopyrroles or cyanothiophene)

RN 78932-45-3 HCAPLUS
CN Cyclopropanecarboxylic acid, 2-butoxy-, ethyl ester (9CI) (CA INDEX NAME)



IT **78932-45-3 635320-14-8 679816-73-0**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of bipyrrolecarboxylates and thienylpyrrolecarboxylates via heterocyclization of alkoxycyclopropanecarboxylates with cyanopyrroles or cyanothiophene)

IT **679816-74-1P 679816-87-6P 679816-90-1P 679816-91-2P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of bipyrrolecarboxylates and thienylpyrrolecarboxylates via

heterocyclization of alkoxycyclopropanecarboxylates with cyanopyrroles or cyanothiophene)

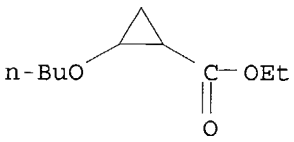
IT **133706-06-6P 679816-75-2P 679816-76-3P 679816-77-4P 679816-78-5P 679816-79-6P 679816-80-9P 679816-83-2P 679816-84-3P 679816-85-4P 679816-86-5P 679816-88-7P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of bipyrrolecarboxylates and thienylpyrrolecarboxylates via heterocyclization of alkoxycyclopropanecarboxylates with cyanopyrroles or cyanothiophene)

RE.CNT 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:960478 HCAPLUS
DN 140:111237
TI A Powerful New Strategy for Diversity-Oriented Synthesis of Pyrroles from Donor-Acceptor Cyclopropanes and Nitriles
AU **Yu, Ming; Pagenkopf, Brian L.**
CS Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX, 78712, USA
SO Organic Letters (2003), 5(26), 5099-5101
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
AB Lewis acid-activated donor-acceptor cyclopropanes react with aliphatic, aromatic, and .alpha.,.beta.-unsatd. nitriles in a novel cascade [3 + 2] dipolar cycloaddn., dehydration, and tautomerization sequence to afford pyrroles in moderate to excellent overall yield. This cost-effective and regiospecific method is ideally suited for the preparation of combinatorial libraries.

IT **78932-45-3**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(diversity-oriented synthesis of pyrroles via Lewis acid-activated cycloaddn./dehydration/tautomerization reactions of various donor-acceptor cyclopropanes and nitriles)

RN 78932-45-3 HCAPLUS
CN Cyclopropanecarboxylic acid, 2-butoxy-, ethyl ester (9CI) (CA INDEX NAME)



IT **78932-45-3 78932-46-4 635320-14-8 647836-52-0**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(diversity-oriented synthesis of pyrroles via Lewis acid-activated cycloaddn./dehydration/tautomerization reactions of various donor-acceptor cyclopropanes and nitriles)

IT **936-12-9P 2199-52-2P 22186-92-1P 27172-04-9P 27188-97-2P 38597-58-9P 647836-43-9P 647836-44-0P 647836-46-2P 647836-48-4P 647836-57-5P 647836-58-6P 647836-59-7P 647836-60-0P 647836-61-1P 647836-62-2P 647836-63-3P 647836-64-4P**

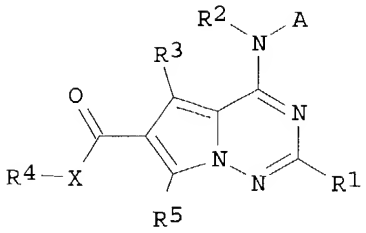
647836-65-5P 647836-66-6P 647836-67-7P
647836-68-8P 647836-69-9P 647836-77-9P
647836-78-0P 647836-79-1P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(diversity-oriented synthesis of pyrroles via Lewis acid-activated cycloaddn./dehydration/tautomerization reactions of various donor-acceptor cyclopropanes and nitriles)
RE.CNT 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d bib abs hitstr hitrn 160 tot

L60 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:875173 HCAPLUS
DN 139:381511
TI Pyrrolotriazine aniline compounds useful as kinase inhibitors, particularly p38 kinases, and their preparation, pharmaceutical compositions, and use as antiinflammatory agents
IN Dyckman, Alaric; Hynes, John; Leftheris, Katherina; Liu, Chunjian; Wrobleski, Stephen T.
PA Bristol-Myers Squibb Company, USA
SO PCT Int. Appl., 158 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003090912	A1	20031106	WO 2003-US12426	20030415 <--
	WO 2003090912	C2	20040108		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2004082582	A1	20040429	US 2003-420399	**20030422** <--
PRAI	US 2002-374938P	P	**20020423** <--		

OS MARPAT 139:381511
GI



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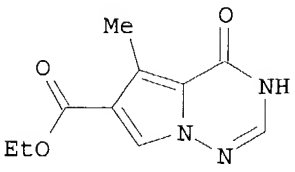
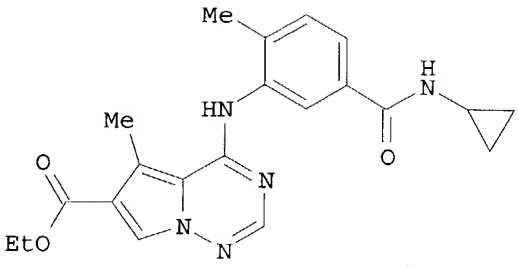


II



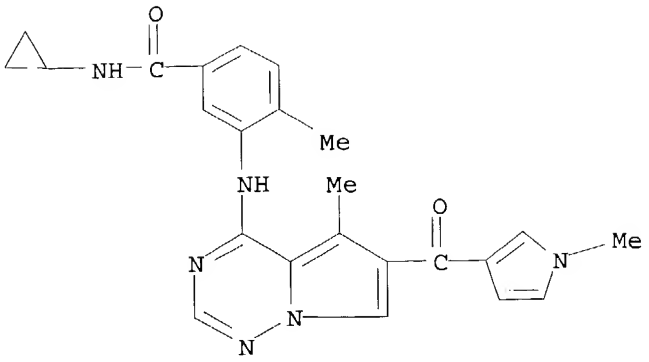
III

AB Title compds. I and their enantiomers, diastereomers, pharmaceutically acceptable salts, prodrugs, and solvates are useful as p38 kinase inhibitors [wherein: A = certain substituted Ph rings, particularly bearing various carboxamide and sulfonamide substituents; X = O, OCO, S, S(O), SO2, CO, CO2, (un)substituted NH, NHCO, NHCONH, NHCO2, NHSO2, NHSO2NH, SO2NH, or CONH, halo, NO2, cyano, or bond; R1, R5 = H, (un)substituted alkyl, OH or derivs., SH or derivs, CO2H or derivs., NH2 or derivs., halo, NO2, cyano; R2 = H, alkyl; R3 = H, Me, CF3, MeO, halo, cyano, NH2, or NHMe; R4 = H (with provisos), (un)substituted alk(en/yn)yl, (hetero)aryl, (hetero)cycloalkyl, or absent]. Over 300 specific compds. I and various intermediates were prepared Compds. I selectively inhibited human p38.alpha./.beta. isoenzymes and TNF-.alpha. in vitro (no data). For instance, 3-amino-4-methylbenzoic acid was amidated quant. with cyclopropylamine using EDC and DMAP in DMF. The pyrrolotriazinone ester II was then chlorinated at the ring oxo group with POCl3 (100%). Aminolysis of the resulting chloride with the benzamide product from the first step gave 80% invention compound III.

IT **623153-04-8P 623153-07-1P**
RL: PAC (Pharmacological activity); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)** ; USES (Uses)
(drug candidate; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

RN 623153-04-8 HCAPLUS

CN Benzamide, N-cyclopropyl-4-methyl-3-[[5-methyl-6-[(1-methyl-1H-pyrrol-3-yl)carbonyl]pyrrolo[2,1-f][1,2,4]triazin-4-yl]amino]- (9CI) (CA INDEX NAME)



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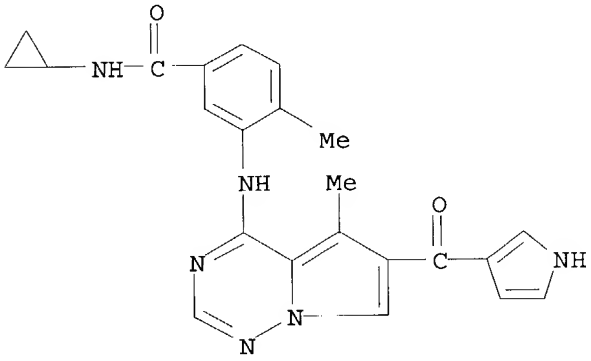
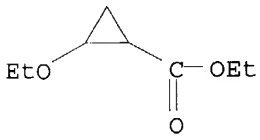


IT **5604-58-0P 53381-05-8P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(intermediate; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)
RN 5604-58-0 HCAPLUS
CN Cyclopropanecarboxylic acid, 2-ethoxy-, ethyl ester (6CI, 9CI) (CA INDEX NAME)



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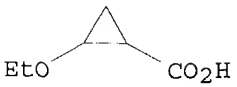
CN Cyclopropanecarboxylic acid, 2-ethoxy- (9CI) (CA INDEX NAME)



IT **623153-04-8P 623153-07-1P**
RL: PAC (Pharmacological activity); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(drug candidate; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

IT **5604-58-0P 53381-05-8P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(intermediate; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FILE 'HCAPLUS' ENTERED AT 11:31:51 ON 14 JUL 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 14 Jul 2004 VOL 141 ISS 3
FILE LAST UPDATED: 13 Jul 2004 (20040713/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d all hitstr l60

L60 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:875173 HCAPLUS
DN 139:381511
ED Entered STN: 07 Nov 2003
TI Pyrrolotriazine aniline compounds useful as kinase inhibitors, particularly p38 kinases, and their preparation, pharmaceutical compositions, and use as antiinflammatory agents
IN Dyckman, Alaric; Hynes, John; Leftheris, Katherina; Liu, Chunjian; Wrobleski, Stephen T.
PA Bristol-Myers Squibb Company, USA
SO PCT Int. Appl., 158 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM B01F003-12
ICS B01F005-26; B01F007-24; B01F007-26; B01F015-02
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
FAN.CNT 1

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GW, ML, MR, NE, SN, TD, TG
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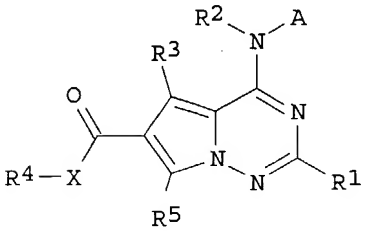

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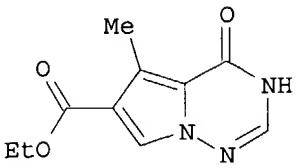

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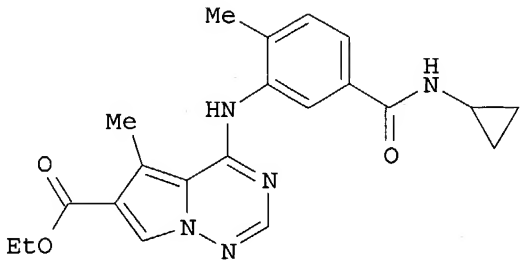

III

AB Title compds. I and their enantiomers, diastereomers, pharmaceutically acceptable salts, prodrugs, and solvates are useful as p38 kinase inhibitors [wherein: A = certain substituted Ph rings, particularly bearing various carboxamide and sulfonamide substituents; X = O, OCO, S, S(O), SO2, CO, CO2, (un)substituted NH, NHCO, NHCONH, NHCO2, NHSO2, NHSO2NH, SO2NH, or CONH, halo, NO2, cyano, or bond; R1, R5 = H, (un)substituted alkyl, OH or derivs., SH or derivs, CO2H or derivs., NH2 or derivs., halo, NO2, cyano; R2 = H, alkyl; R3 = H, Me, CF3, MeO, halo, cyano, NH2, or NHMe; R4 = H (with provisos), (un)substituted alk(en/yn)yl, (hetero)aryl, (hetero)cycloalkyl, or absent]. Over 300 specific compds. I and various intermediates were prepared Compds. I selectively inhibited human p38.alpha./.beta. isoenzymes and TNF-.alpha. in vitro (no data). For instance, 3-amino-4-methylbenzoic acid was amidated quant. with cyclopropylamine using EDC and DMAP in DMF. The pyrrolotriazinone ester II was then chlorinated at the ring oxo group with POCl3 (100%). Aminolysis of the resulting chloride with the benzamide product from the first step gave 80% invention compound III.

ST aniline pyrrolotriazine prepn p38 kinase inhibitor; anilinopyrrolotriazine prepn kinase TNF alpha inhibitor antiinflammatory

IT Respiratory distress syndrome
(adult, treatment; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

IT Antiarteriosclerotics
(antiatherosclerotics; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

IT Lung, disease
(chronic inflammation, treatment; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

IT Lung, disease

(chronic obstructive, treatment; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

IT Transplant and Transplantation
(graft-vs.-host reaction, treatment; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

IT Intestine, disease
(inflammatory, treatment; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

IT Tumor necrosis factors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

IT Anti-inflammatory agents
Antiarthritics
Antiasthmatics
Antidiabetic agents
Human
(preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

IT Arthritis
(psoriatic arthritis, treatment; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

IT Arthritis
(traumatic, treatment; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

IT Gout
Rubella
(treatment of associated arthritis; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

IT Arthritis
Asthma
Atherosclerosis
Diabetes mellitus
Inflammation
Osteoarthritis
Osteoporosis
Psoriasis
Rheumatoid arthritis
(treatment; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

IT 623152-12-5P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

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RL: PAC (Pharmacological activity); **SPN (Synthetic preparation)**;
THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**
; USES (Uses)
(drug candidate; preparation of pyrrolotriazine aniline compds. as p38
kinase inhibitors)

IT 623154-51-8P 623154-52-9P 623154-53-0P 623154-54-1P 623154-55-2P
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(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(drug candidate; preparation of pyrrolotriazine aniline compds. as p38
kinase inhibitors)

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623155-61-3P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(intermediate; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

IT 165245-96-5, p38 Kinase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

IT 62-53-3, Aniline, reactions 75-31-0, Isopropyl amine, reactions 78-81-9, Isobutyl amine 78-96-6 85-41-6, Phthalimide 96-50-4, 2-Aminothiazole 96-54-8, 1-Methylpyrrole 99-55-8, 2-Methyl-5-nitroaniline 100-58-3, Phenylmagnesium bromide 100-66-3, Anisole, reactions 107-10-8, 1-Propanamine, reactions 109-01-3, 1-Methylpiperazine 109-04-6, 2-Bromopyridine 109-55-7, N,N-Dimethyl-1,3-propanediamine 109-73-9, 1-Butanamine, reactions 109-85-3 109-89-7, Diethylamine, reactions 109-92-2, Ethyl vinyl ether 109-97-7, 1H-Pyrrole 110-00-9, Furan 110-85-0, Piperazine, reactions 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 119-32-4, 4-Methyl-3-nitroaniline 120-72-9, 1H-Indole, reactions 123-00-2, 4-Morpholinepropanamine 123-62-6, Propionic anhydride 123-75-1, Pyrrolidine, reactions 124-40-3, Dimethylamine, reactions 151-18-8 155-09-9 156-87-6, 3-Amino-1-propanol 288-13-1, Pyrazole 288-32-4, Imidazole, reactions 372-47-4, 3-Fluoropyridine 402-67-5, 3-Fluoronitrobenzene 403-54-3, 3-Fluorobenzonitrile 504-24-5, 4-Aminopyridine 504-29-0, 2-Aminopyridine 513-49-5 585-79-5, 3-Bromonitrobenzene 603-76-9, 1-Methyl-1H-indole 616-45-5, 2-Pyrrolidinone 618-61-1, 3-Nitro-5-methylaniline 622-47-9, p-Tolylacetic acid 623-73-4, Ethyl diazoacetate 765-30-0, Cyclopropylamine 826-85-7 933-88-0, 2-Methylbenzoyl chloride 1448-87-9, 2-Chloroquinoxaline 1750-42-1, 3-Aminoisoxazole 1820-80-0, 3-Amino-1H-pyrazole 2038-03-1, 4-Morpholineethanamine 2265-94-3, 3,5-Difluoronitrobenzene 2458-12-0 2516-47-4, Cyclopropylmethanamine 2620-50-0, 1,3-Benzodioxole-5-methanamine 2627-86-3 3524-32-1 3731-51-9, 2-Pyridinemethanamine 3731-52-0, 3-Pyridinemethanamine 3731-53-1, 4-Pyridinemethanamine 4005-51-0, 1,3,4-Thiadiazol-2-amine 4442-59-5 4570-45-0, 2-Aminooxazole 4572-03-6 5036-48-6, 1H-Imidazole-1-propanamine 5332-73-0, 3-Methoxy-1-propanamine 5333-27-7 5382-16-1, 4-Piperidinol 5805-57-2, 1H-Benzimidazole-2-methanamine 6291-85-6, 3-Ethoxy-1-propanamine 6627-60-7 7154-73-6, 1-Pyrrolidineethanamine 7175-81-7 7202-43-9 7305-71-7 10397-30-5, 3-Nitro-4-methylbenzoyl chloride 19013-11-7 20010-99-5, Pyrazinemethanamine 23159-07-1, 1-Pyrrolidinepropanamine 51387-90-7 56613-80-0 65287-34-5, 2-Chloro-4-pyridinecarbonyl chloride 74370-93-7 75985-45-4, 2-Pyrimidinemethanamine 84540-59-0, 4-Methyl-3-nitrobenzyl chloride 105919-28-6 118430-73-2 129714-97-2, 3,5-Difluorobenzoyl chloride 250681-75-5 317806-86-3 387350-39-2 427877-76-7 427878-02-2 427878-70-4 621685-64-1 623155-62-4 623155-63-5 623155-64-6 623155-65-7 623155-66-8

RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

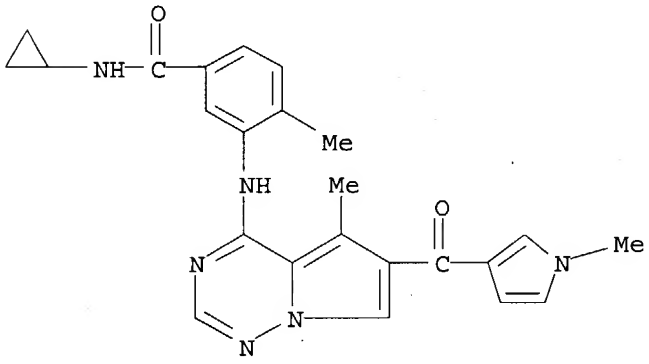
RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

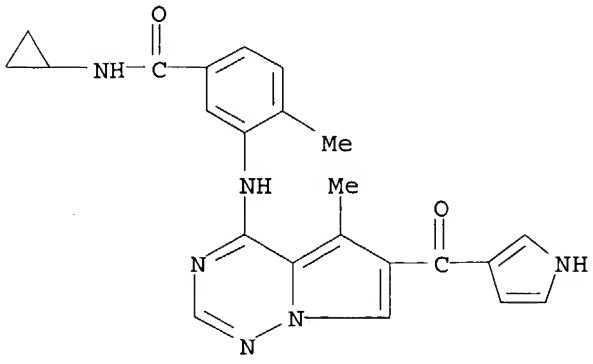
(1) Johansson; US 4824032 A 1989
(2) Kirschbraun; US 1560826 A 1925 HCAPLUS
(3) O'Brein; US 5478147 A 1995
(4) Pillon; US 4883363 A 1989
(5) Schneider; US 4955723 A 1990

IT **623153-04-8P 623153-07-1P**
RL: PAC (Pharmacological activity); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(drug candidate; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

RN 623153-04-8 HCAPLUS
CN Benzamide, N-cyclopropyl-4-methyl-3-[[5-methyl-6-[(1-methyl-1H-pyrrol-3-yl)carbonyl]pyrrolo[2,1-f][1,2,4]triazin-4-yl]amino]- (9CI) (CA INDEX NAME)



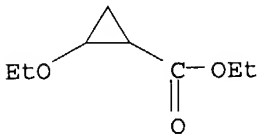
RN 623153-07-1 HCAPLUS
CN Benzamide, N-cyclopropyl-4-methyl-3-[[5-methyl-6-(1H-pyrrol-3-ylcarbonyl)pyrrolo[2,1-f][1,2,4]triazin-4-yl]amino]- (9CI) (CA INDEX NAME)



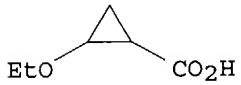
IT **5604-58-0P 53381-05-8P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP

(Preparation); **RACT (Reactant or reagent)**
(intermediate; preparation of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

RN 5604-58-0 HCAPLUS
CN Cyclopropanecarboxylic acid, 2-ethoxy-, ethyl ester (6CI, 9CI) (CA INDEX NAME)



RN 53381-05-8 HCAPLUS
CN Cyclopropanecarboxylic acid, 2-ethoxy- (9CI) (CA INDEX NAME)



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